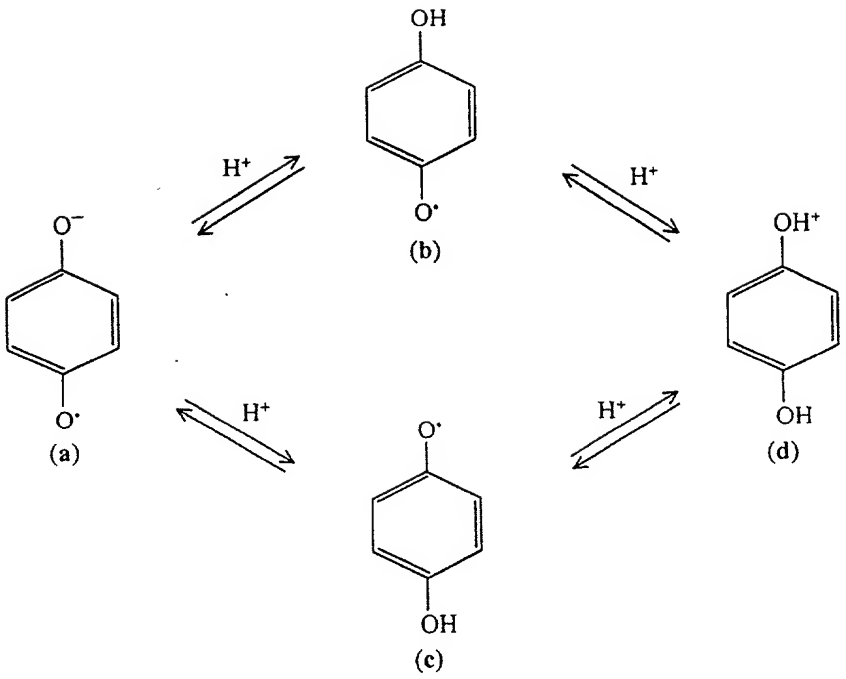


Fig 1. Mesomeric forms of p-benzosemiquinone. (a) anionic; (b),(c) neutral; (d) cationic.

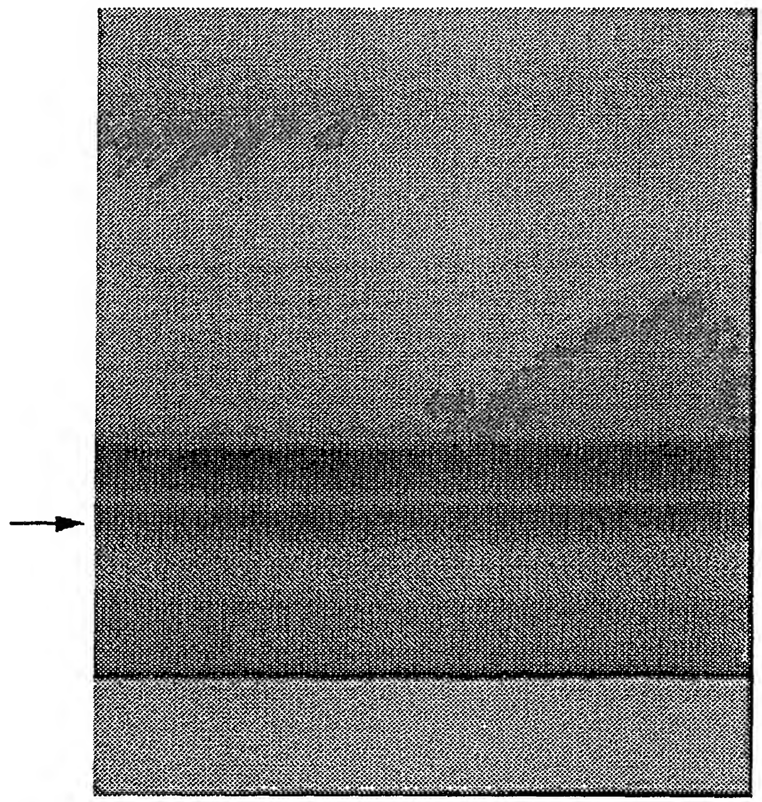


Fig 2. Band thin layer chromatography of the methanol solution after lyophilization (step 5). ⟶ Indicates the band of cs-oxidant.

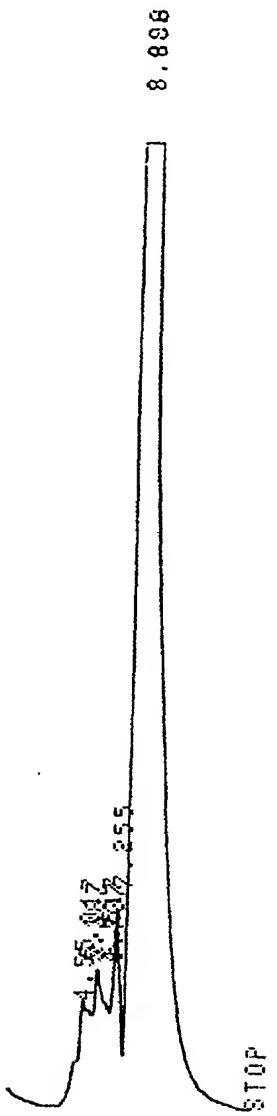


Fig 3. HPLC profile the butanol extract after TLC. The cs-oxidant (step 6) eluted as a major peak at the retention time of 8.808 min. The amount of cs-oxidant eluted was ≈ 12 μg.

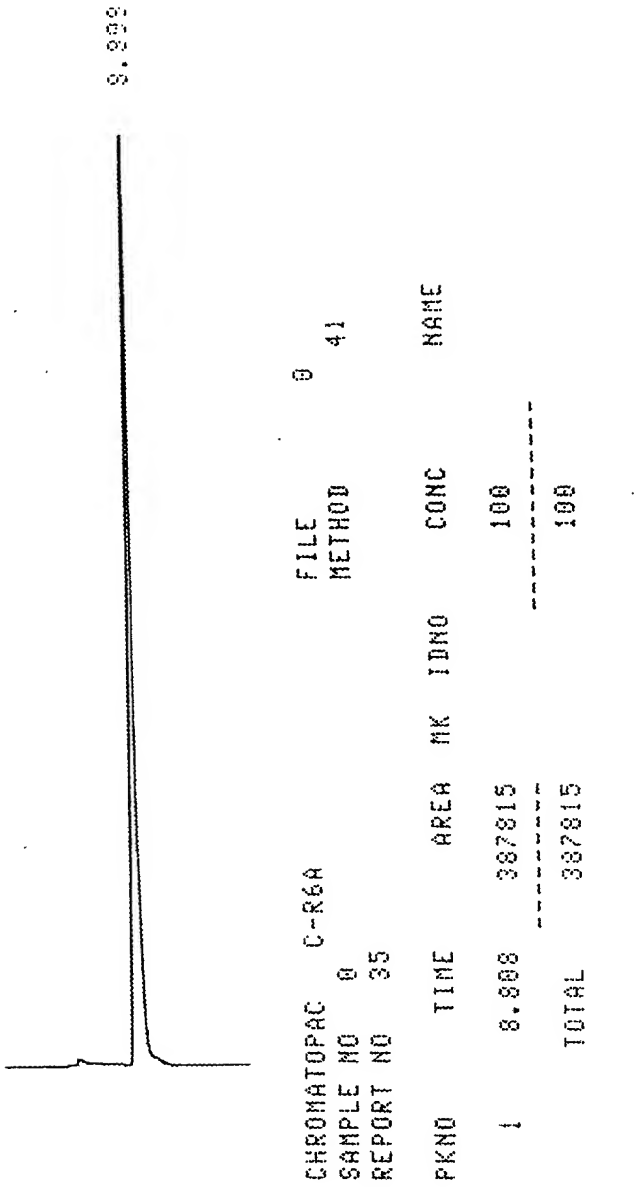


Fig 4. HPLC profile of the pure cs-oxidant, eluted at the retention time of 8.808 min.

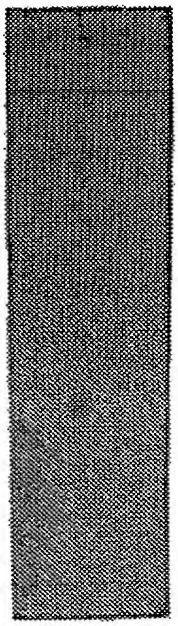


Fig 5. Thin layer chromatography of the pure cs-oxidant (R_f= 0.26)

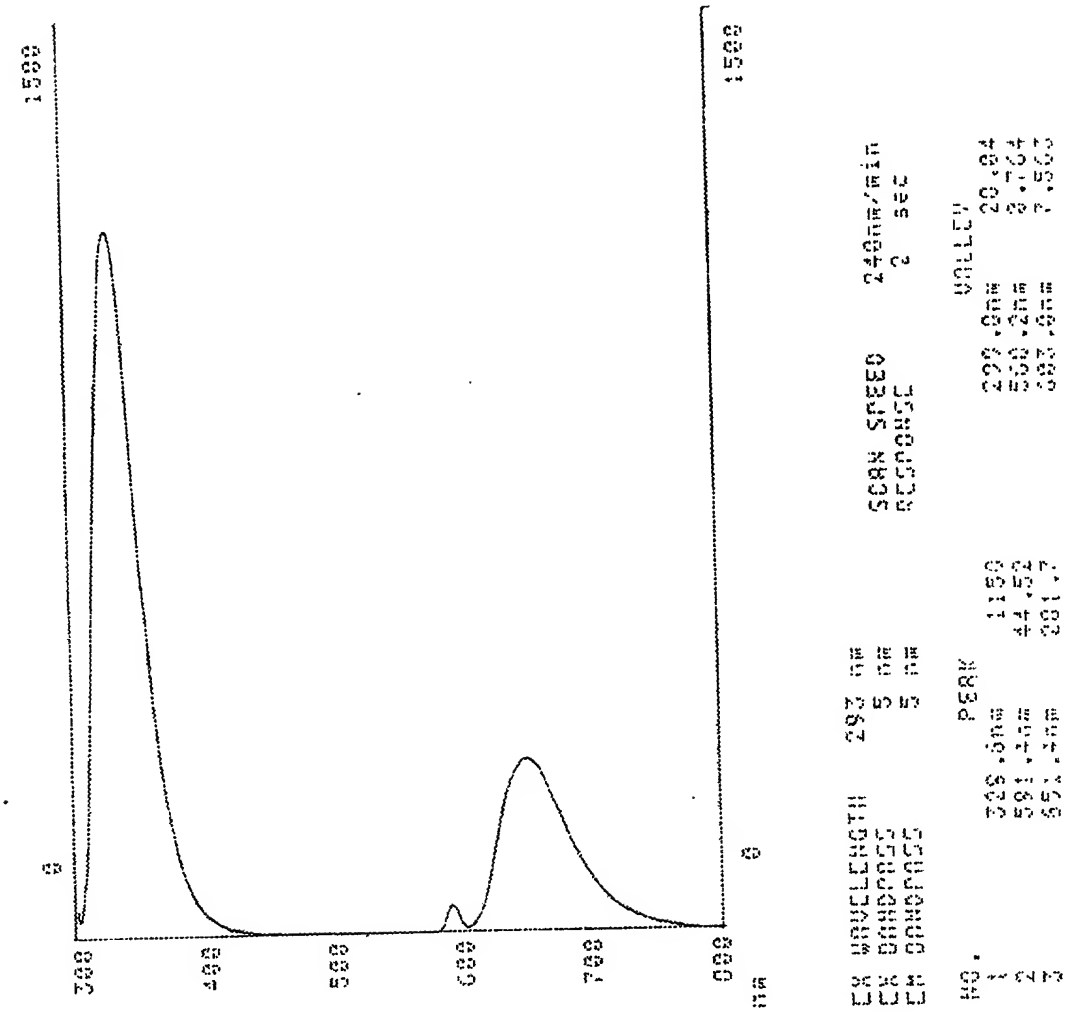


Fig 6a. Fluorescence spectroscopic profile of the cs-oxidant in methanol. The excitation was at 293 nm and the emission scanning was measured from 300 nm to 800 nm. The emission maxima were at 329.6 nm and at 651.4 nm.

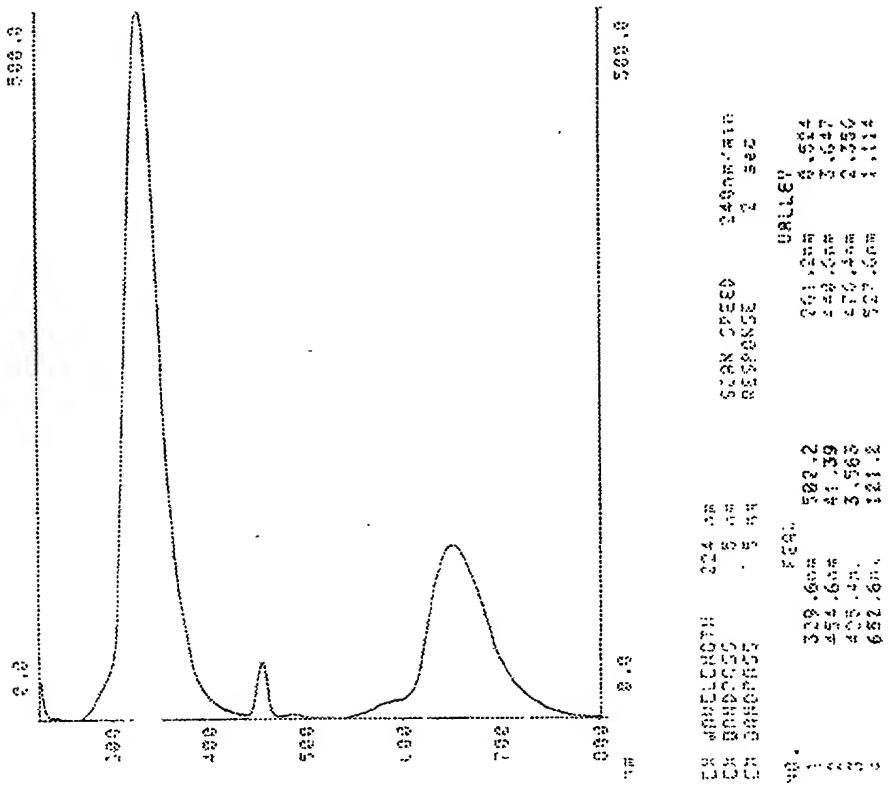


Fig 6b Fluorescence spectroscopic profile of the cs-oxidant in methanol The excitation was at 224 nm and the emission scanning was measured from 225 nm to 800 nm. The emission maxima were at 329 6 nm and at 652 6 nm.

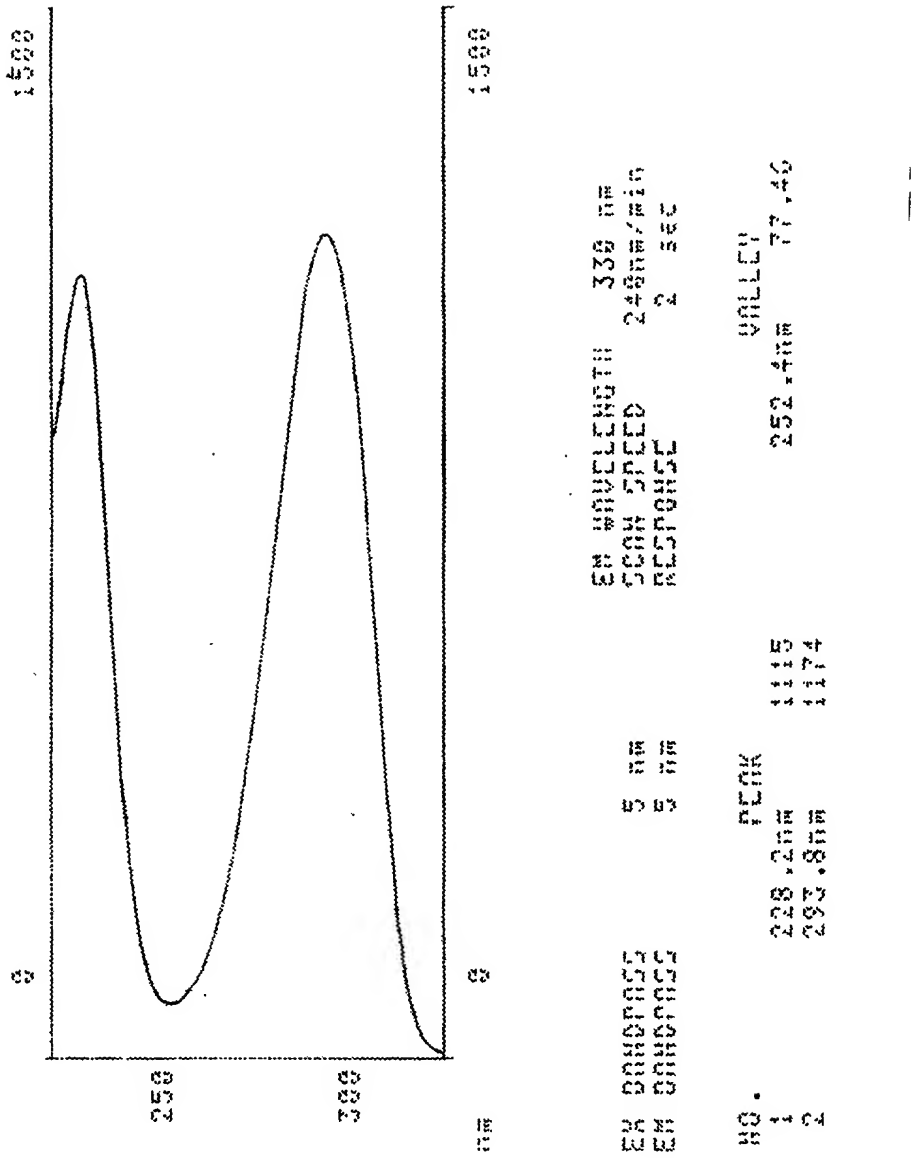


Fig 7a. Fluorescence spectroscopic profile of the cs-oxidant in methanol. The emission was at 330 nm and the excitation scanning was measured from 220 nm to 325 nm. The excitation maxima were at 228.2 nm and at 293.8 nm.

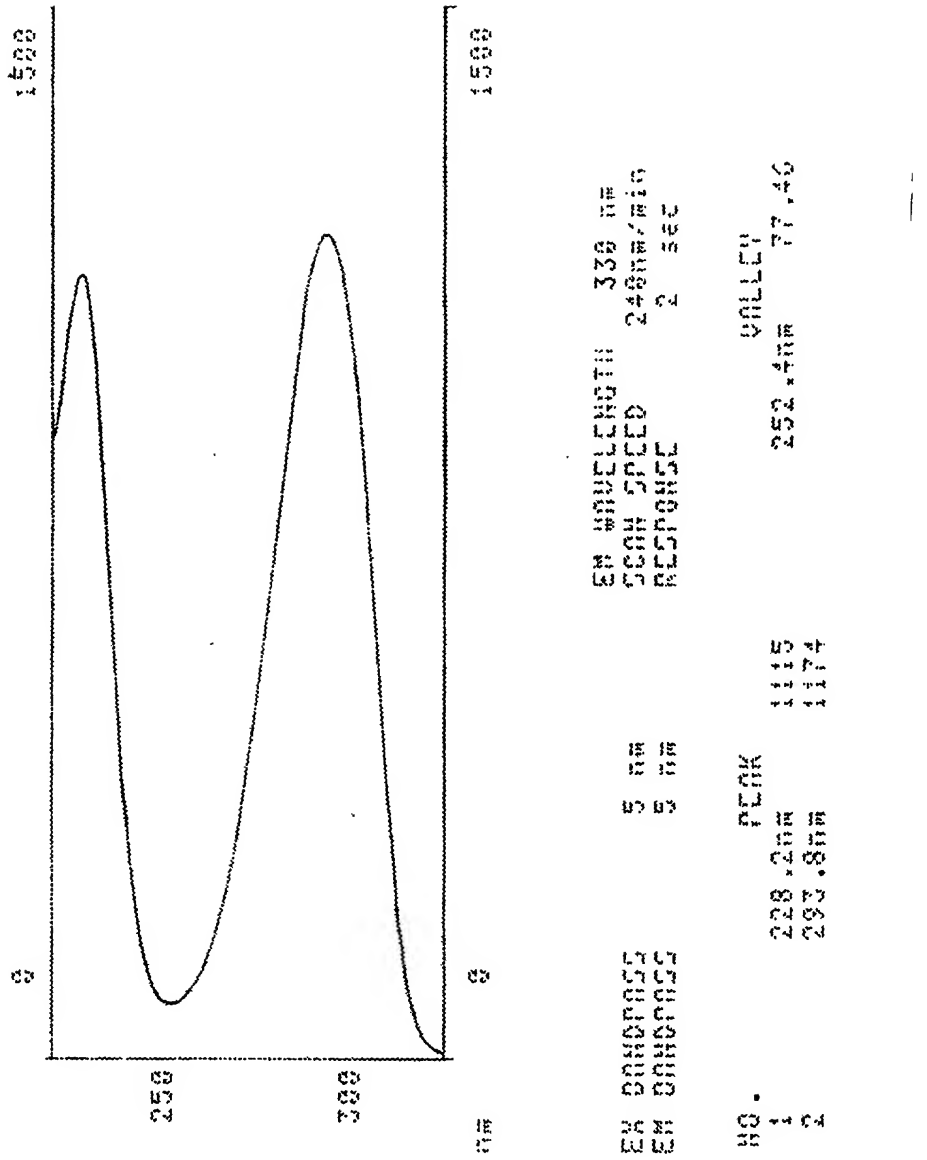


Fig 7a. Fluorescence spectroscopic profile of the cs-oxidant in methanol. The emission was at 330 nm and the excitation scanning was measured from 220 nm to 325 nm. The excitation maxima were at 228.2 nm and at 293.8 nm.

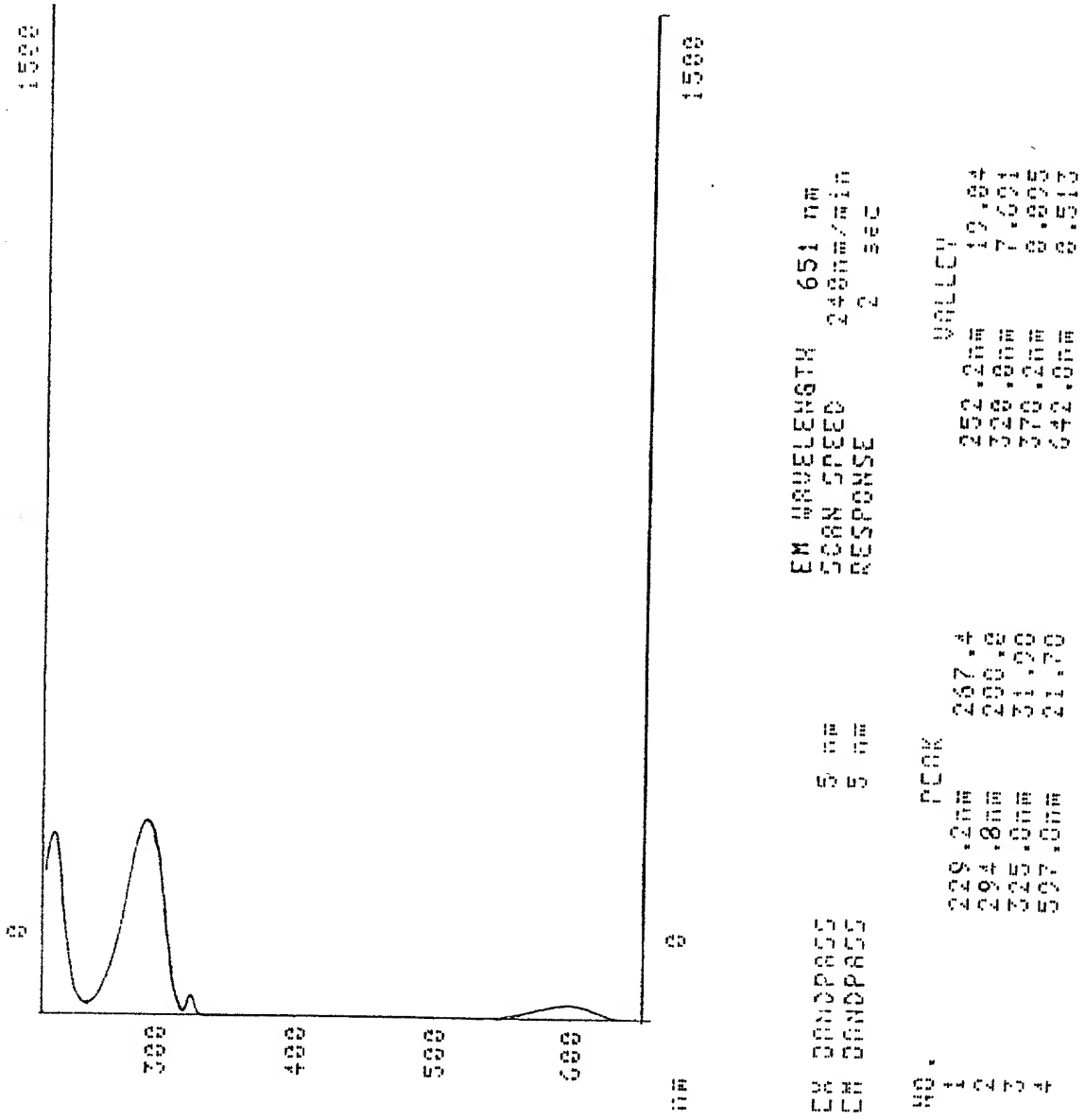


Fig 7b. Fluorescence spectroscopic profile of the cs-oxidant in methanol. The emission was at 651 nm and the excitation scanning was measured from 220 nm to 650 nm. The excitation maxima were at 229.2 nm and at 294.8 nm.

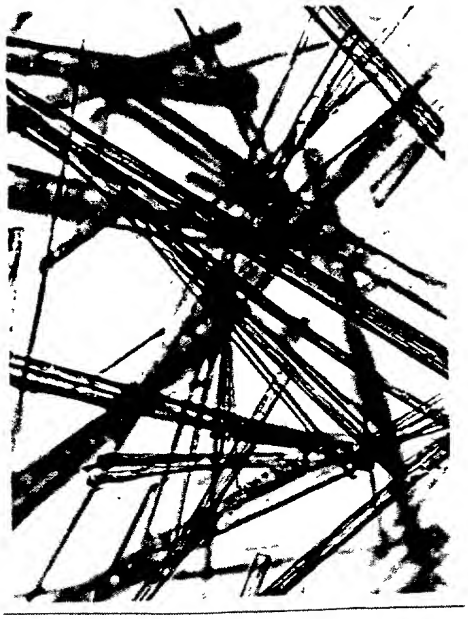


Fig 8. Crystal structure of the pure cs-oxidant

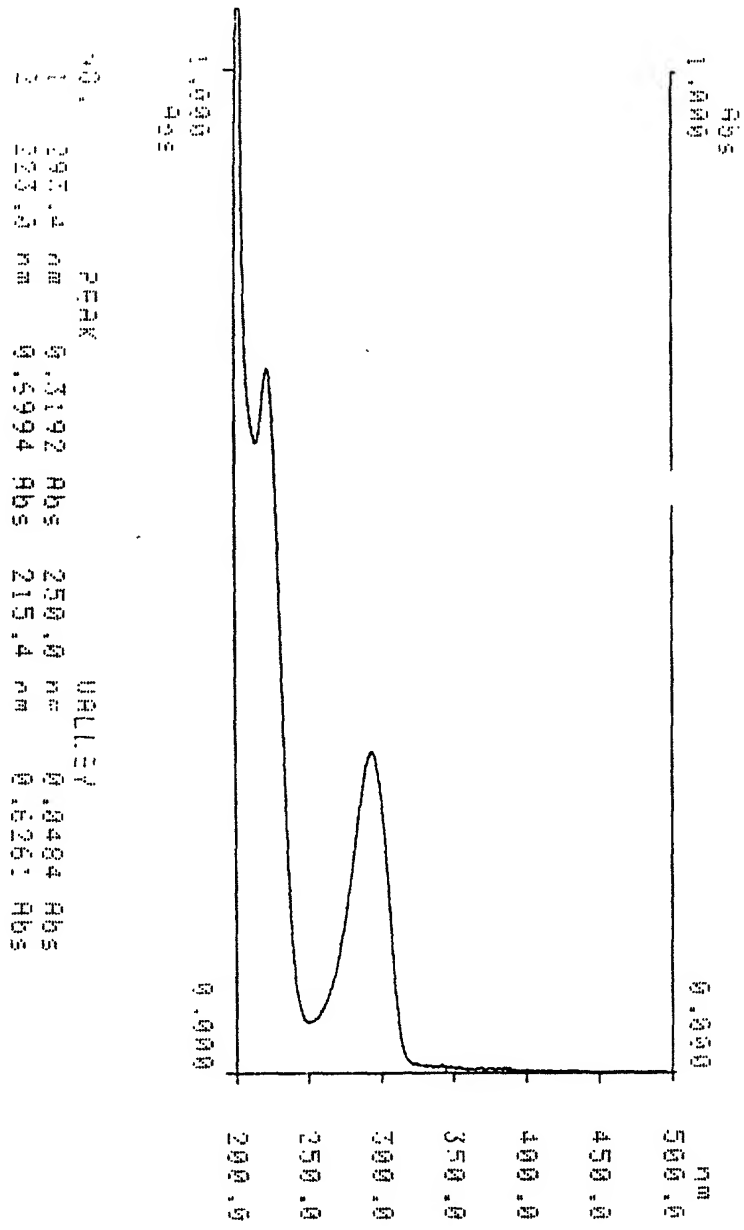


Fig 9. UV spectrophotometric profile of the cs-oxidant in methanol. It has two absorption maxima, one at 293.4 nm and another at 223.0 nm.

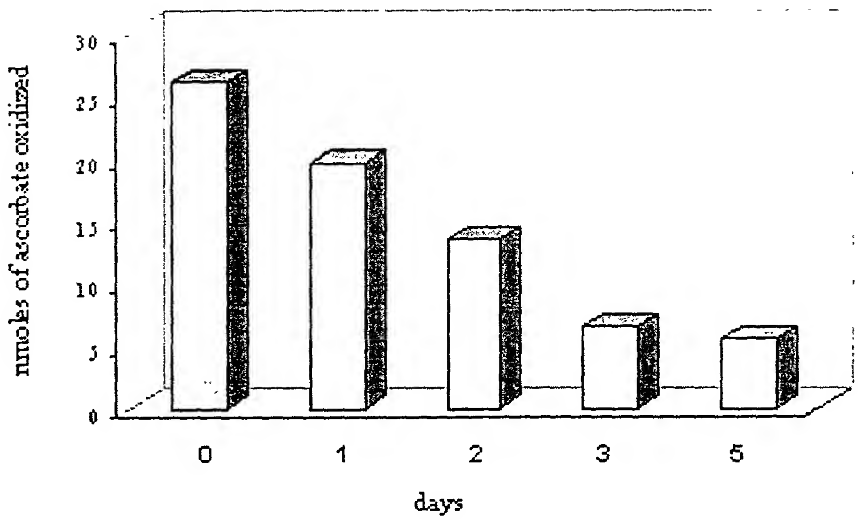


Fig.10 Stability of the solid oxidant kept at 25°C under darkness. The stability was determined by its capacity to oxidize ascorbic acid. Ascorbic acid was measured by HPLC analysis at 254 nm.

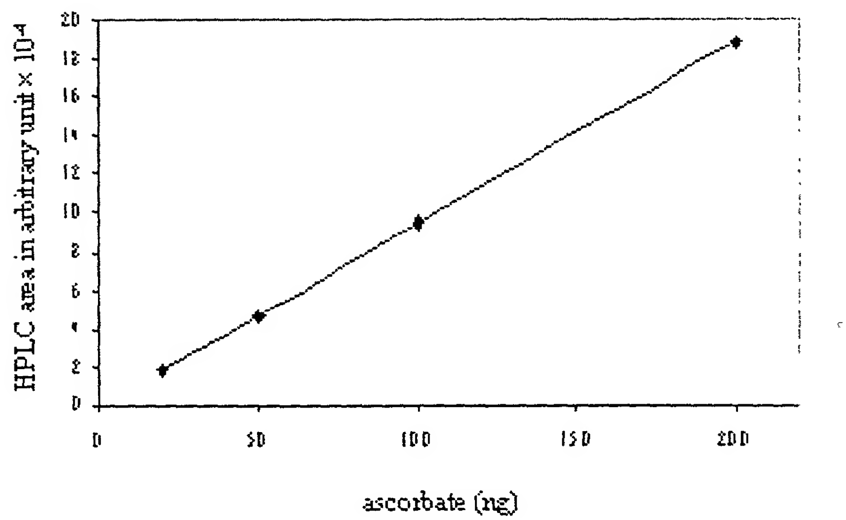


Fig.11 Standard curve of ascorbic acid based on HPLC analysis at 254 nm.

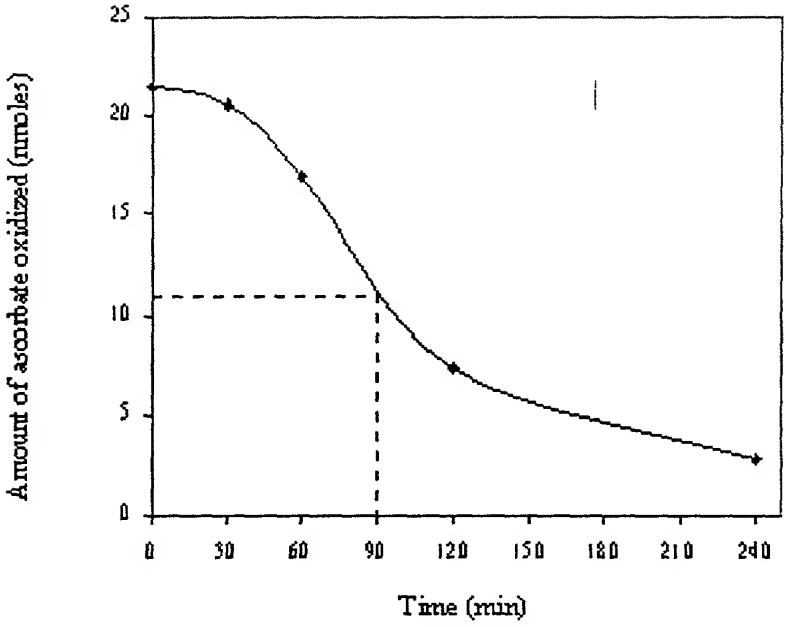


Fig.12 Stability of the cs-oxidant in 50 mM potassium phosphate buffer at 25°C measured by its potency to oxidize ascorbate as evidenced by HPLC area.

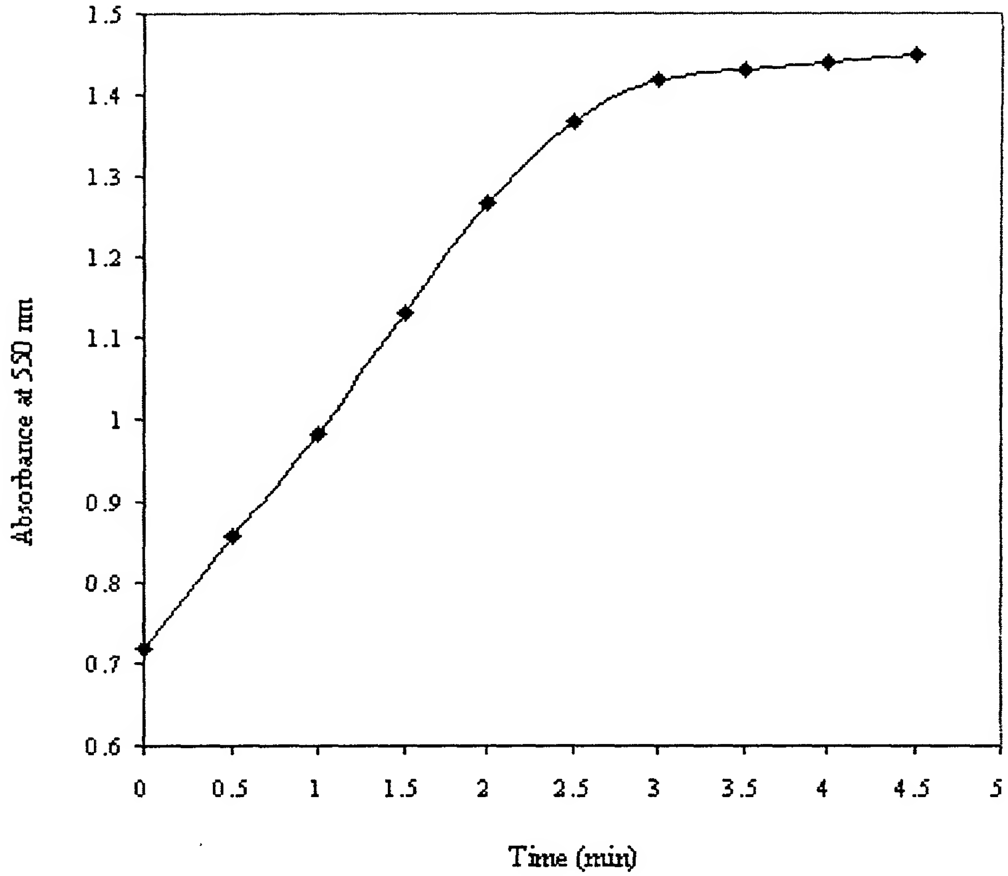


Fig.13 Quantitative reduction of ferricytochrome c by the oxidant as measured by the formation of ferrocytochrome c with time at 550 nm. The reaction was carried out in 50 mM potassium phosphate buffer, pH 7.4, keeping the final concentration of ferricytochrome c at 100μM. One nmole of the oxidant reduced 0.71 nmoles of ferricytochrome c.

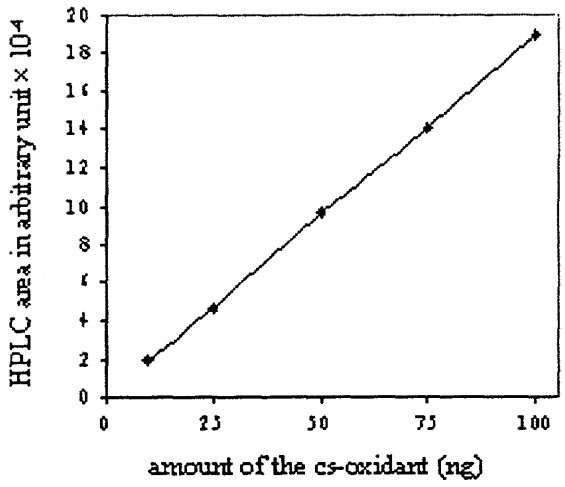


Fig 14. Standard curve of the oxidant on the basis of HPLC area at 294 nm. Different amounts of the cs-oxidant were used ranging from 10 ng to 100 ng in 20µl of mobile solvent.

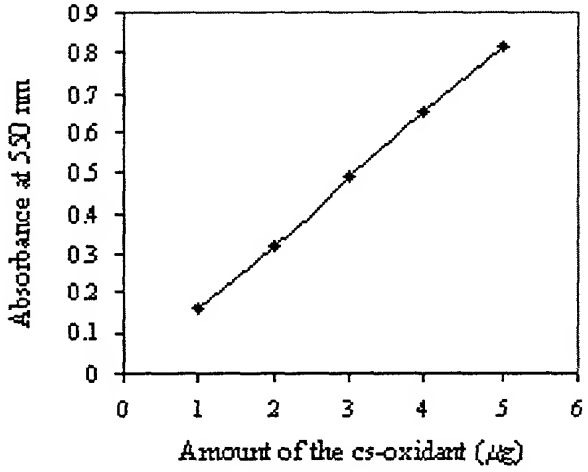


Fig 15. Standard curve of the oxidant on the basis of reduction of cytochrome c by using different amounts of the oxidant ranging from 1µg to 5 µg.

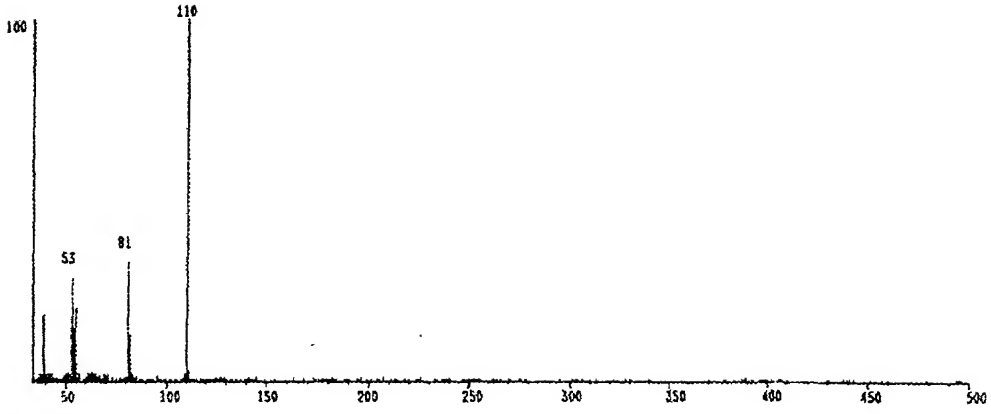


Fig 16. Mass spectrum of the pure cs-oxidant

Fig 17. UV spectrophotometric profile of the hydroquinone in methanol. It has two absorption maxima, one at 293.8 nm and another at 224.2 nm.

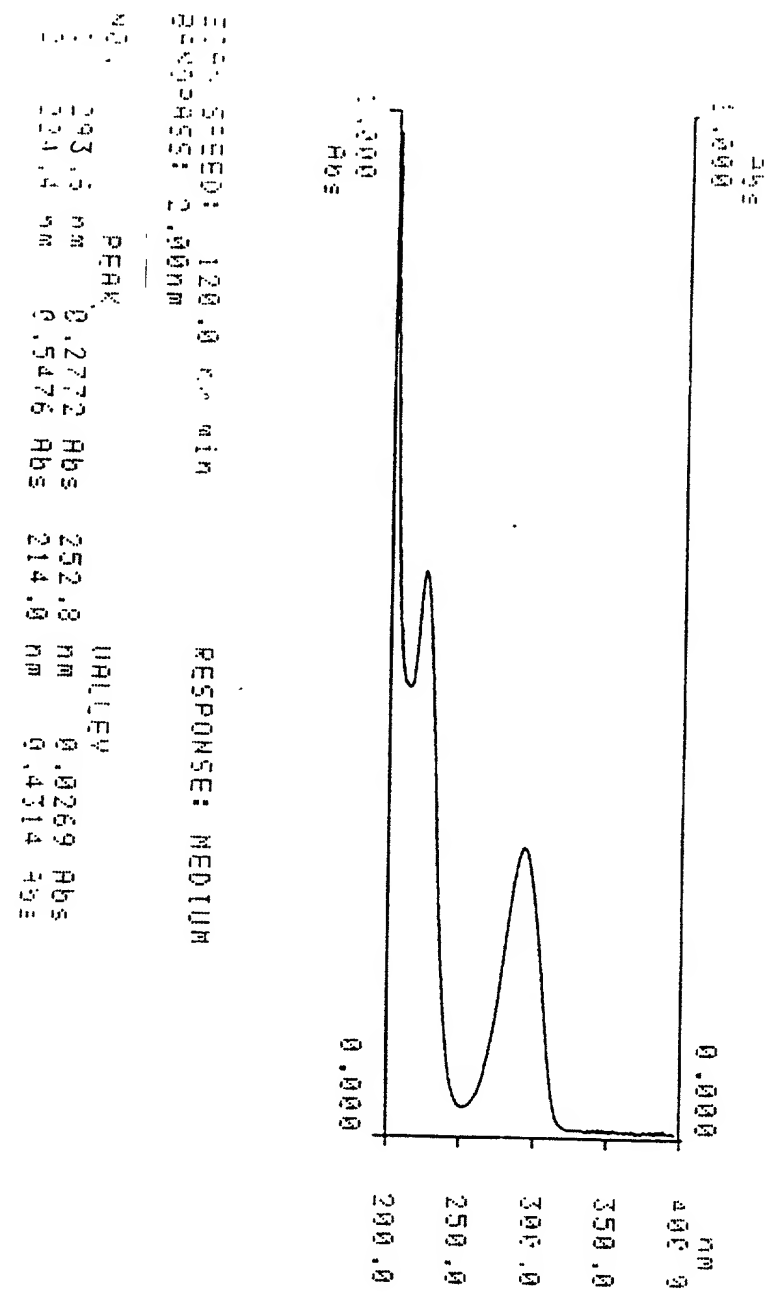


Fig 18. UV spectrophotometric profile of the cs-oxidant stored at room temperature in dark for 8 days. The two absorption maxima are at 293.6 nm and at 224.4 nm.

Fig 19. UV spectrophotometric profile of equimolar mixture of p-benzoquinone and hydroquinone in methanol. There is a shoulder near 242 nm (the λ_{max} of p-benzoquinone).

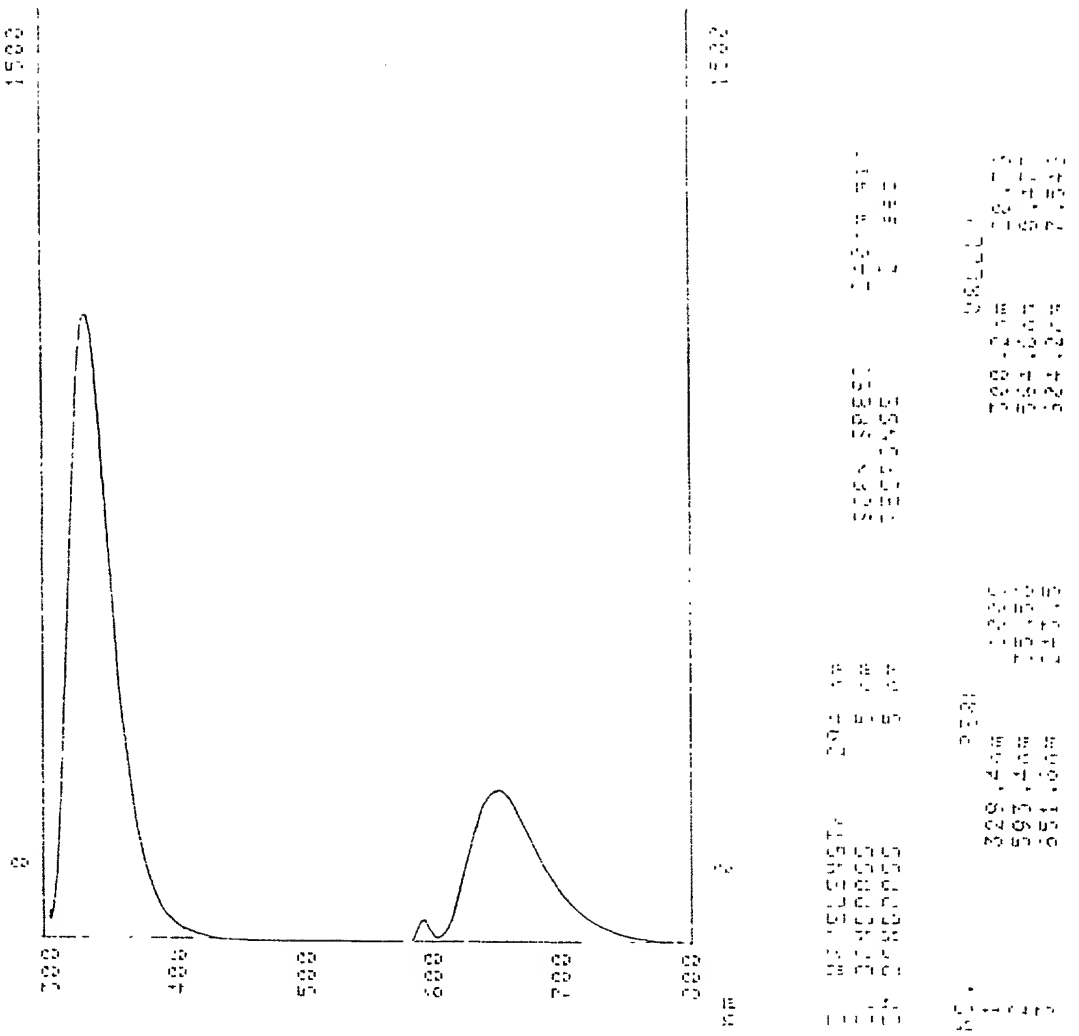


Fig 20. Fluorescence spectroscopic profile of the hydroquinone in methanol The excitation was at 294 nm and the emission scanning was measured from 300 nm to 800 nm. The emission maxima were at 329.4 nm and at 651.6 nm.

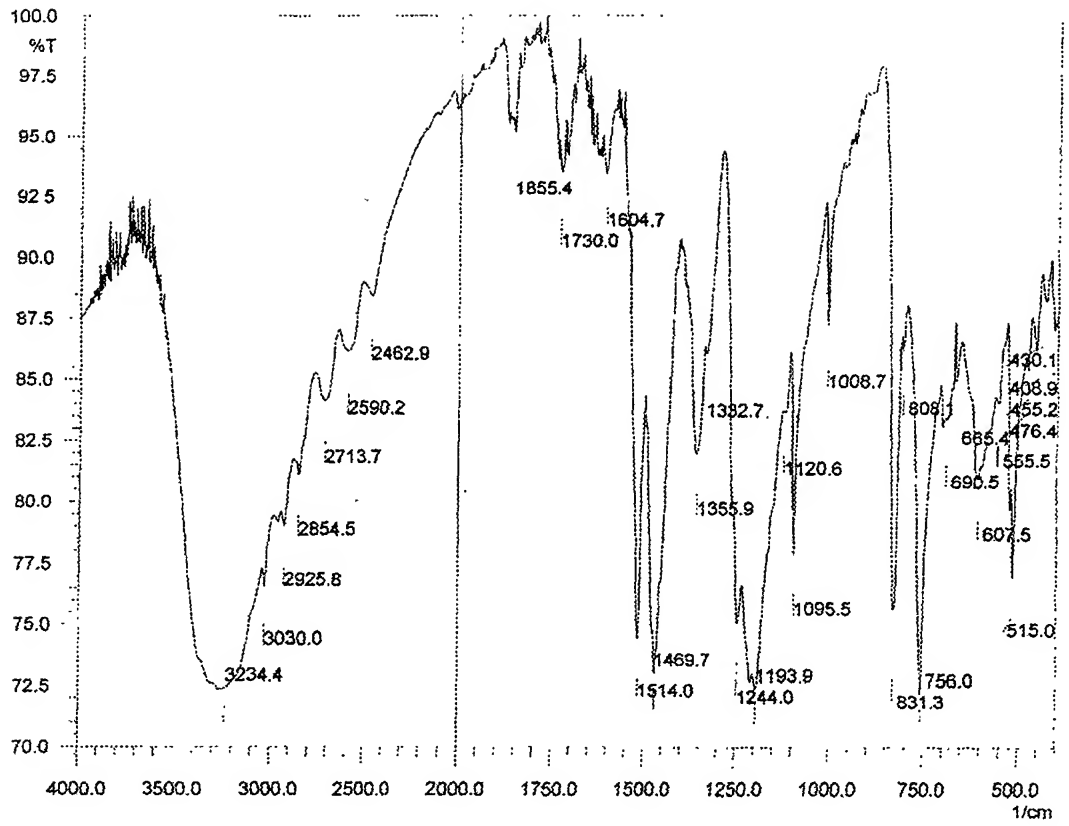


Fig 21. FTIR spectroscopic profile of the cs-oxidant.

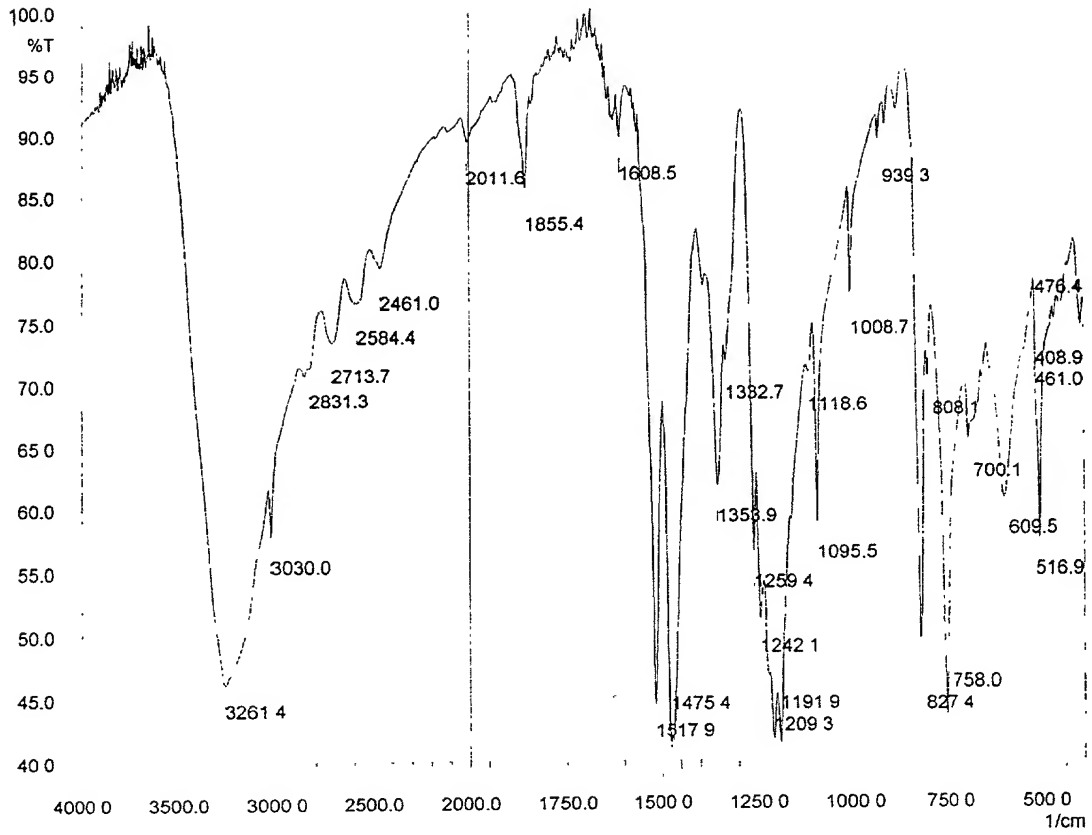


Fig 22 FTIR spectroscopic profile of hydroquinone

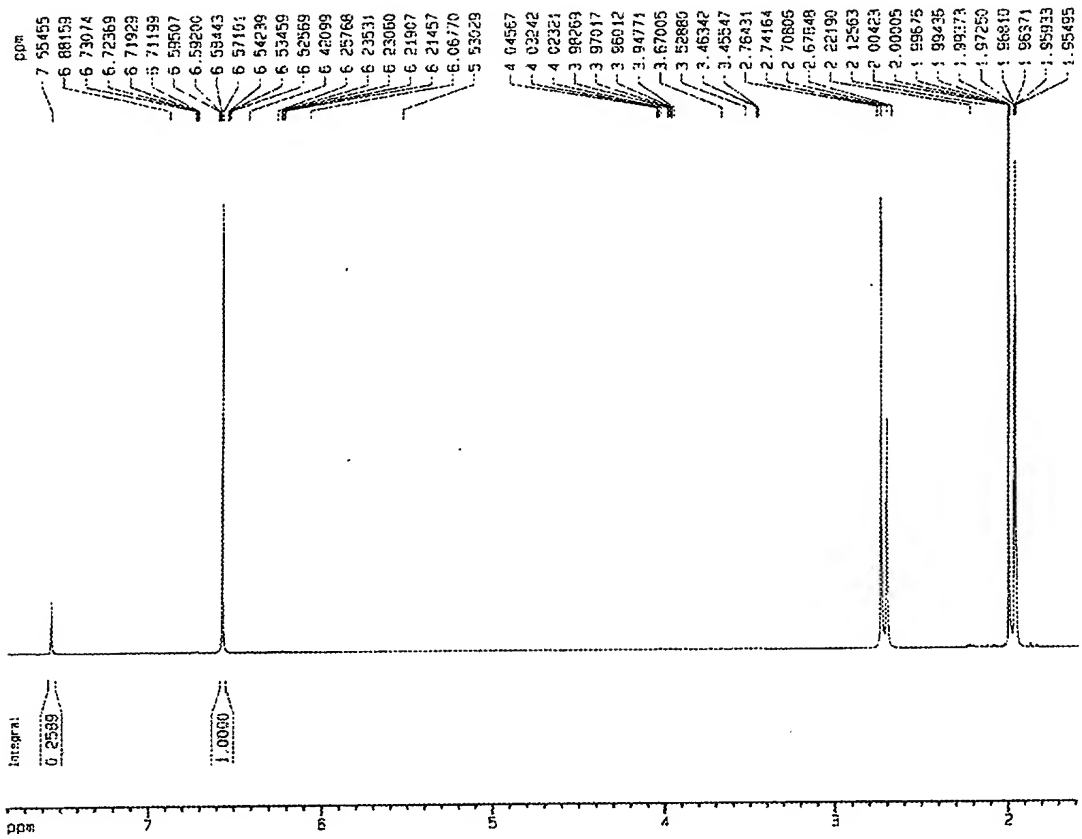


Fig 23 H-NMR spectroscopic profile of the cs-oxidant in CD_3COCD_3

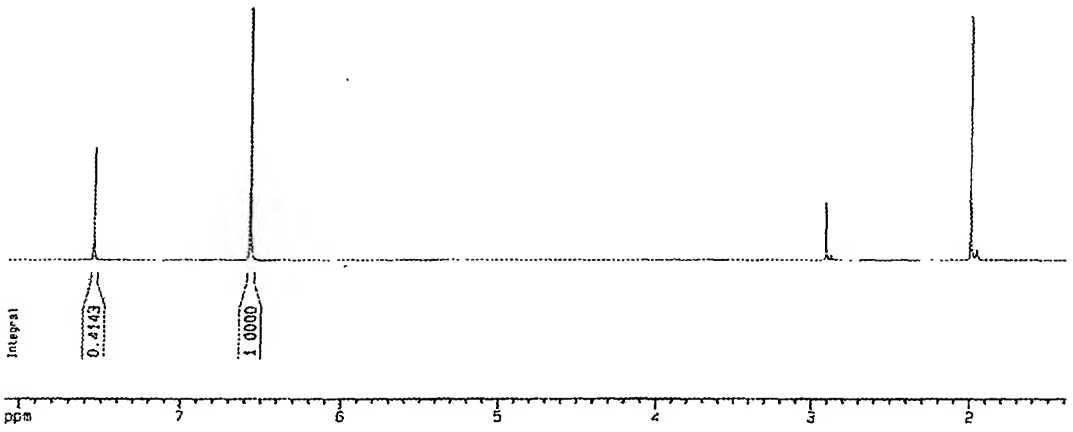


Fig 24. H-NMR spectroscopic profile of hydroquinone in CD_3COCD_3

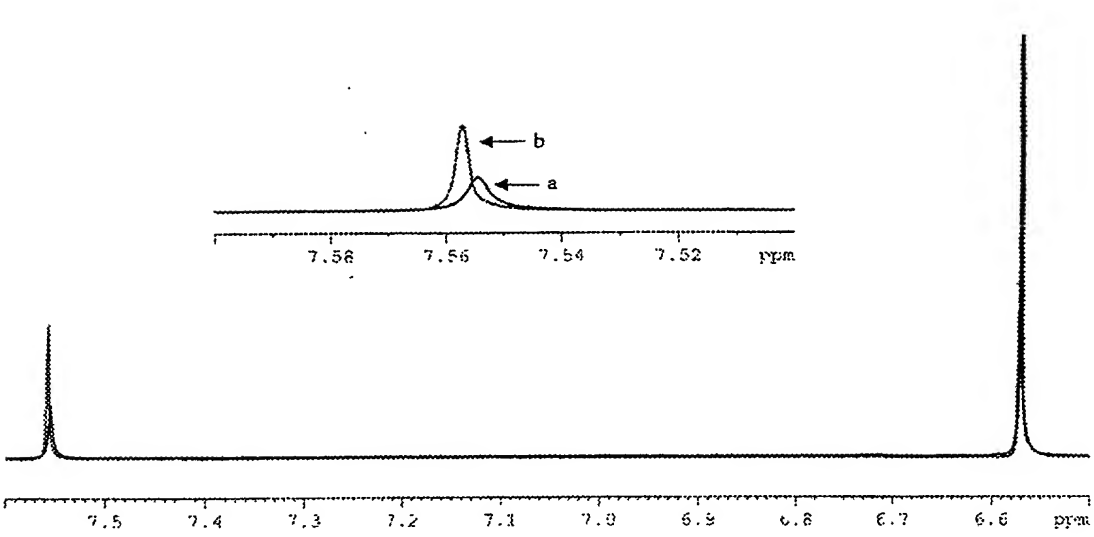


Fig 25 Comparative H-NMR spectroscopic profiles of (a) cs-oxidant and (b) hydroquinone.

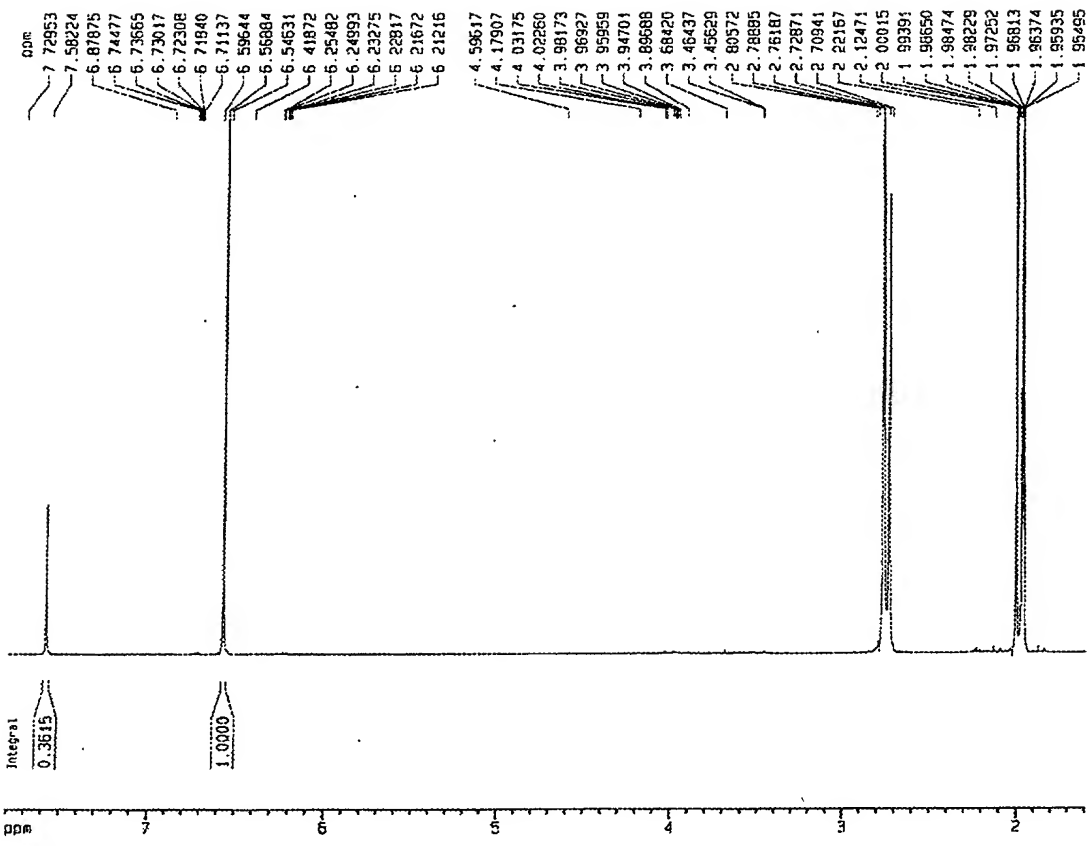


Fig 26. H-NMR spectroscopic profile of the cs-oxidant after reduction with sodium dithionite.

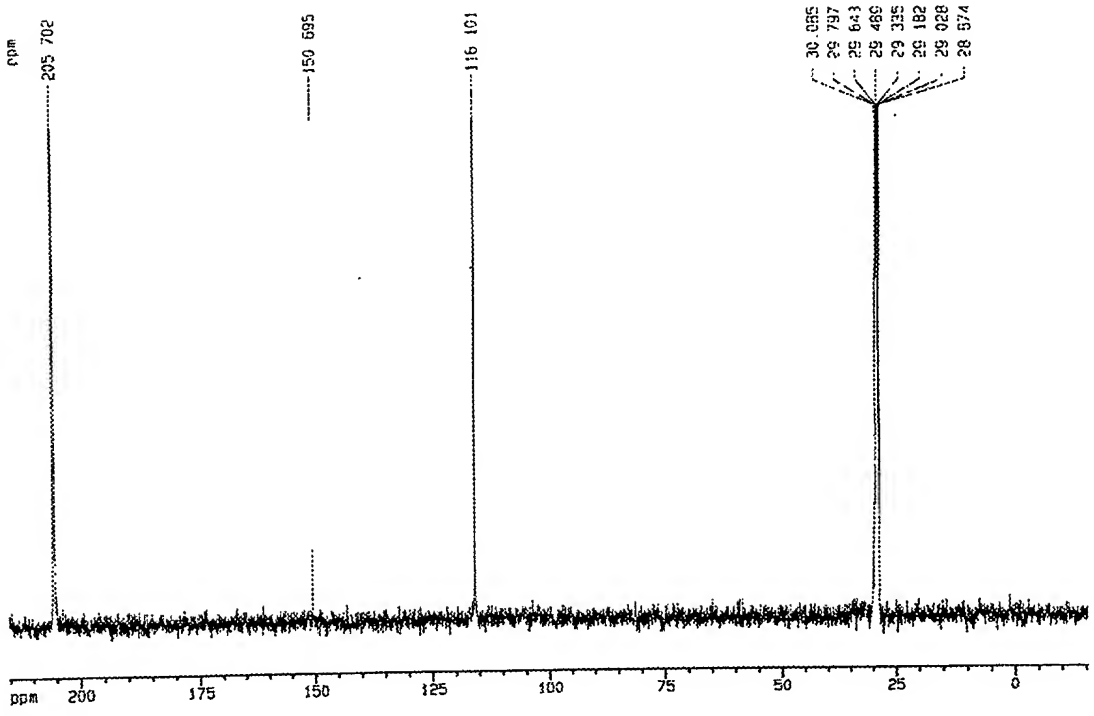


Fig 27 C-NMR spectroscopic profile of the cs-oxidant in CD_3COCD_3

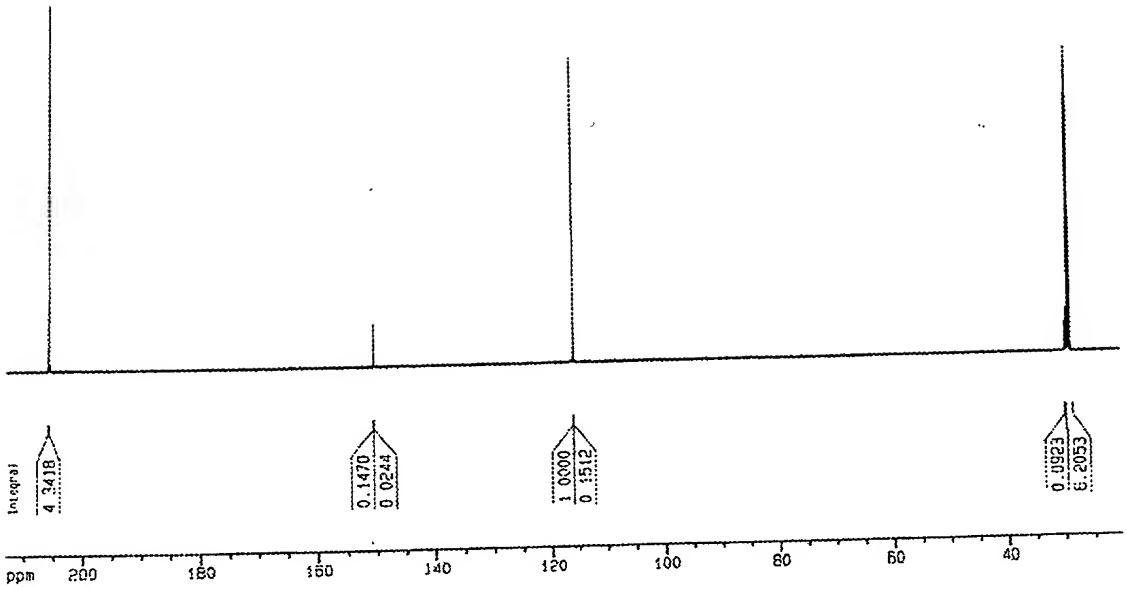


Fig 28. C-NMR spectroscopic profile of hydroquinone in CD_3COCD_3

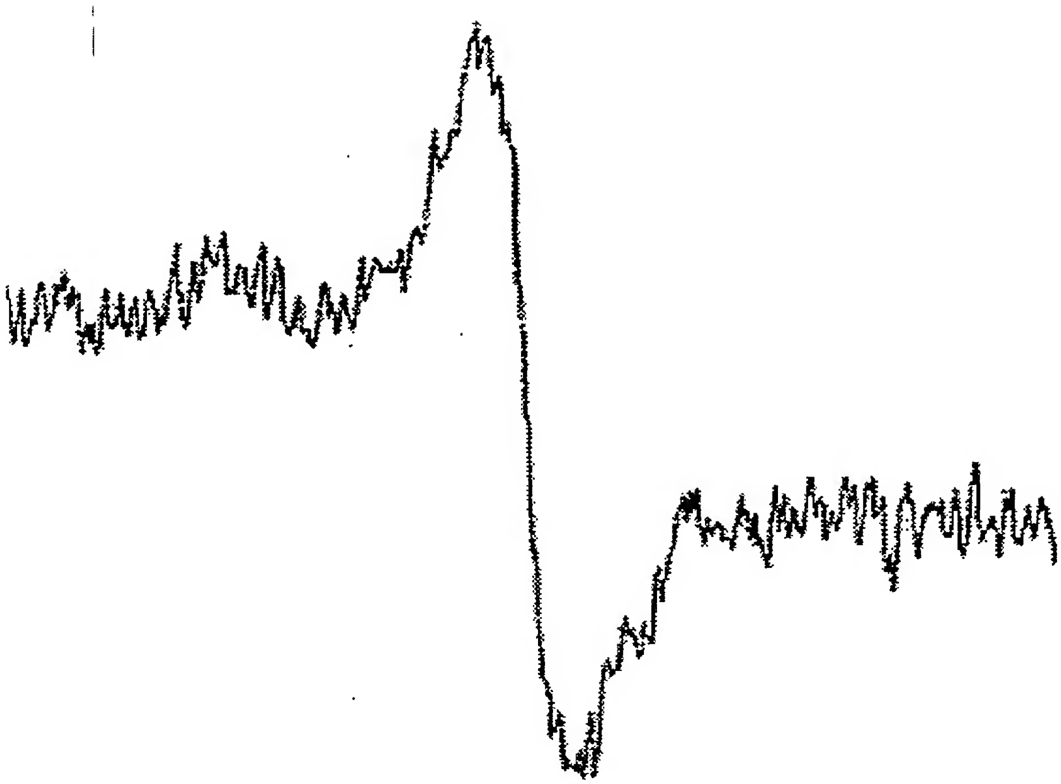


Fig 29. Room temperature ESR spectrum of CS-oxidant, freshly prepared from 100 cigarettes. The spectrum was recorded on a JES-REIX ESR spectrometer (Tokyo, Japan). The spectral parameters were as follows: microwave frequency, 9.435 GHz; power, 2mW; field modulation width, 0.4mT; modulated frequency, 100kHz; time constant, 0.3 sec; scan rate, 2.5 mT/ sec

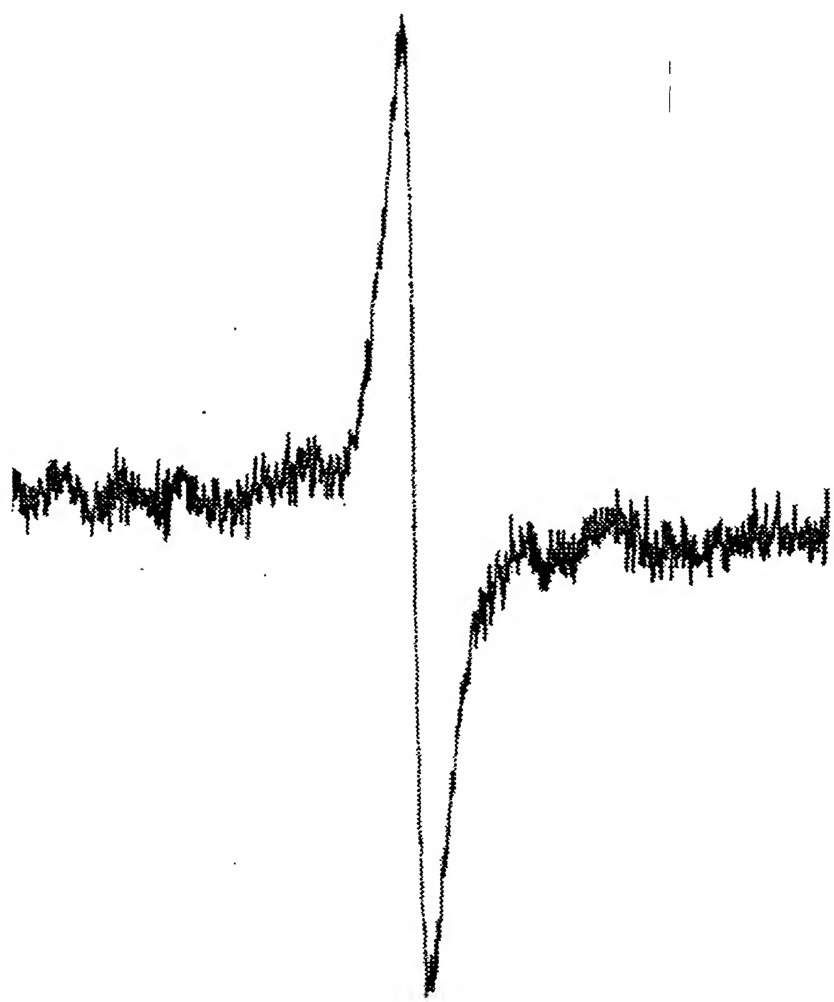


Fig 30. Room temperature ESR spectrum of aged (10 days) cs-oxidant, prepared from 400 cigarettes

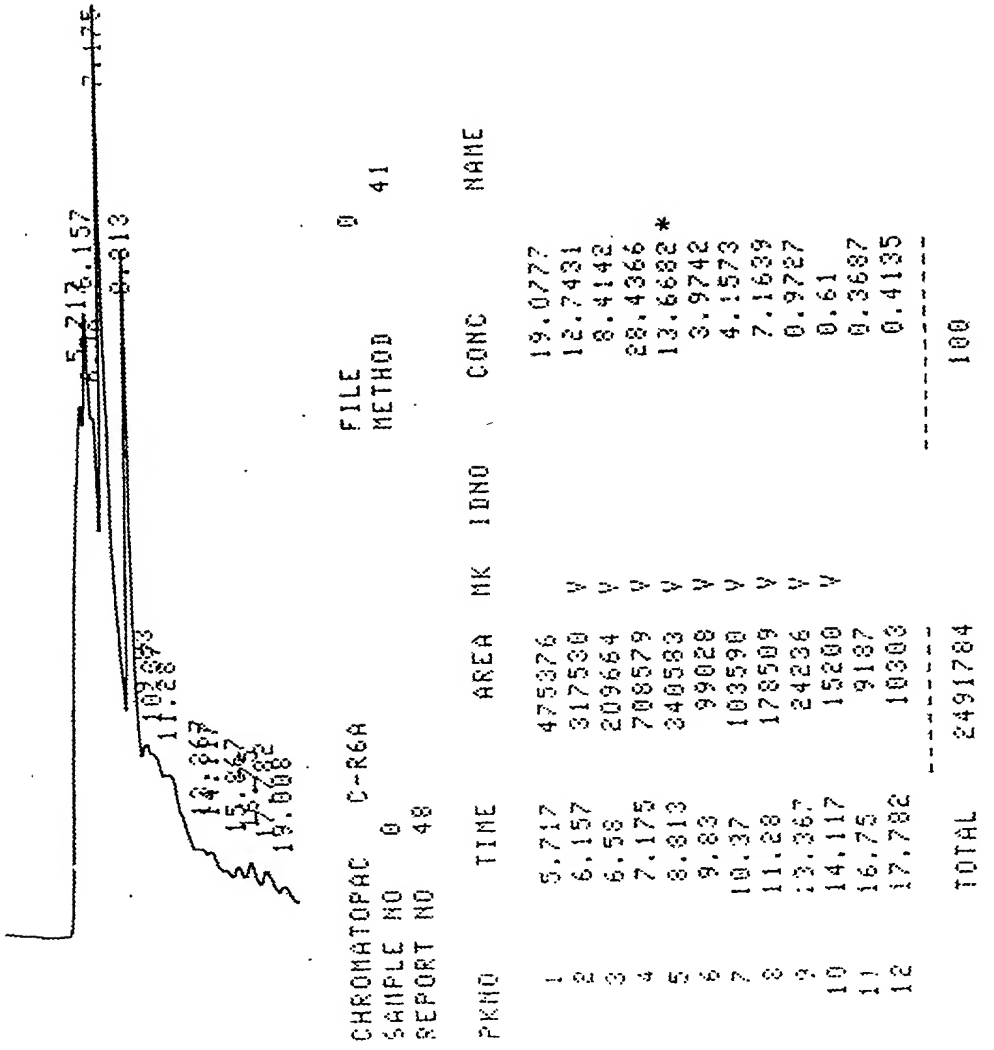
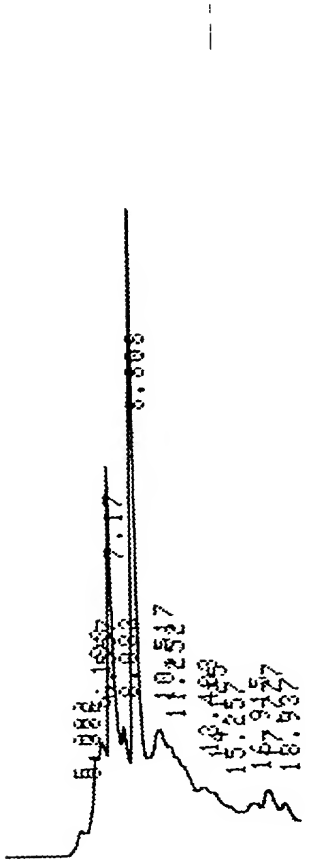


Fig 31. HPLC profile of the whole cs solution analyzed in the silica column (Lichrospher® Si 60, Merck).

* Indicates the retention time, area and the concentration (13.6682%) of the cs-oxidant



CHROMATOPAC C-R6A FILE 0
SAMPLE NO 0 METHOD 41
REPORT NO 47

PKNO	TIME	AREA	MK	IDNO	CONC	NAME
1	5.092	6469			0.5956	
2	6.183	43150	V		3.9726	
3	6.557	54830	V		5.048	
4	7.17	190600	V		17.5478	
5	8.083	59275	V		5.4572	
6	8.808	295731	V		27.2269	*
7	10.517	137178	V		12.6295	
8	11.252	129369	V		11.9105	
9	13.483	39852	V		3.669	
10	14.125	37368	V		3.4403	
11	15.257	16282	V		1.499	
12	16.915	28634	V		2.6362	
13	17.777	32483	V		2.9906	
14	18.937	14954	V		1.3768	
TOTAL		1086173			100	

Fig 32. HPLC profile of the aqueous extract of cs solution analyzed in the silica column (Lichrospher® Si 60, Merck).

* Indicates the retention time, area and the concentration (27.2269%) of the cs-oxidant

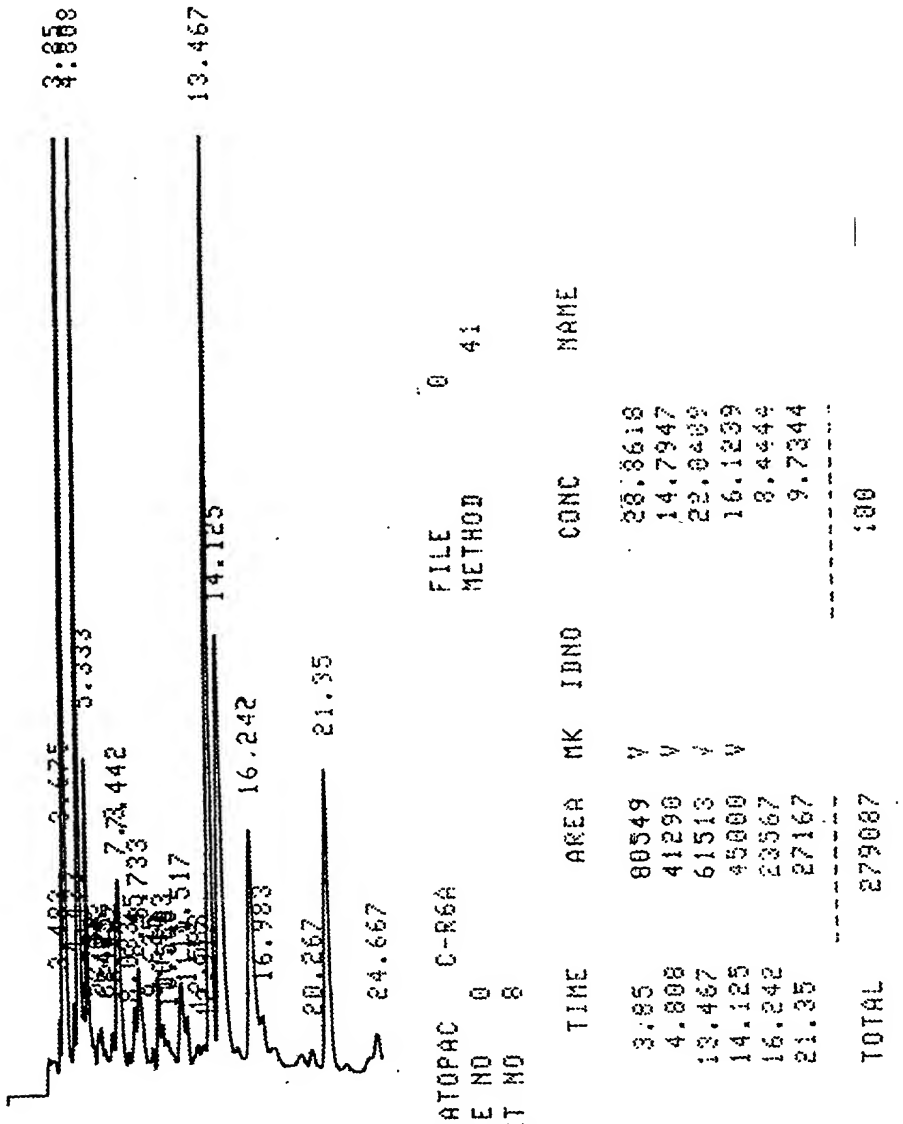


Fig 33. HPLC profile of the whole cs solution analyzed in the ODS column (Shim-pack CLC-ODS, Shimadzu). The cs-oxidant eluted at 13.467 min.

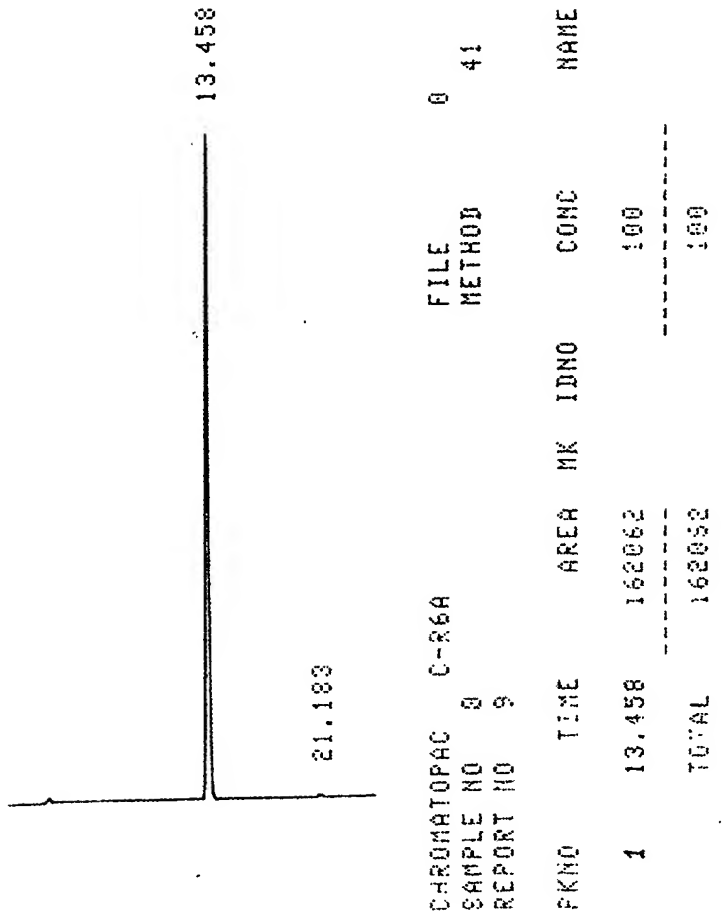


Fig 34. HPLC profile of the pure cs-oxidant, analyzed in the ODS column (Shim-pack CLC-ODS, Shimadzu) eluted at the retention time of 13.458 min.

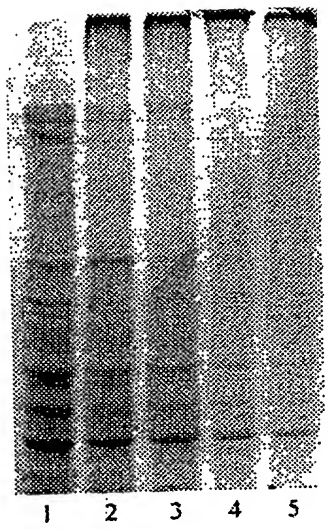


Fig 35a. SDS-PAGE of the guinea pig lung microsomal proteins treated with whole cs solution and the cs-oxidant. Lane 1, untreated microsomes; lane 2, microsomes treated with 50 µl cs solution; lane 3, microsomes treated with 100 µl cs solution; lane 4, microsomes treated with 10µg cs-oxidant; lane 5, microsomes treated with 20µg cs-oxidant.

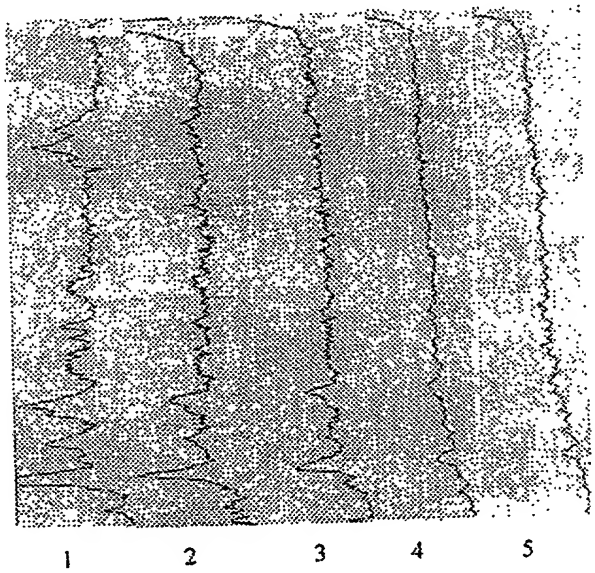


Fig 35b. Densitometric scanning of the protein bands of different lanes as in Fig 35a.